

2,2,8-Trimethyl-7-prop-2-ynoxychromene
94244-29-8 | DTXSID10241225

Model Performance

Model

Data

Weighted KNN model					
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 11.0

Global applicability domain: Inside

Local applicability domain index: 4.64e-01

Confidence level: 6.00e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 219</div> <div>Predicted: 151</div>	<div>Image not found</div> <div>O,O-Diethyl dithiophosphate</div> <div>Measured: 5.01</div> <div>Predicted: 5.43</div>	<div>Image not found</div> <div>Isophorone</div> <div>Measured: 2.00</div> <div>Predicted: 3.19</div>
<div>Image not found</div> <div>Thiram</div> <div>Measured: 3.39</div> <div>Predicted: 3.91</div>	<div>Image not found</div> <div>Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>	<div>Image not found</div> <div>(1R,2S,5R)-(-)-Menthol</div> <div>Measured: 10.8</div> <div>Predicted: 23.5</div>